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Quantum-classical crossover in the spin 1/2 XXZ chain

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Abstract

We compute, by means of exact diagonalization of systems of $N = 16$ and 18 spins, the correlation function $< \sigma_0^z \sigma_n^z >$ at nonzero temperature for the XXZ model with anisotropy Δ. In the gapless attractive region $-1 < \Delta < 0$ for fixed separation the temperature can always be made sufficiently low so that the correlation is always negative for $n \neq 0$. However we find that for sufficiently large temperatures and fixed separation or for fixed temperature greater than some $T_0(\Delta)$ and sufficiently large separations the correlations are always positive. This sign changing effect has not been previously seen and we interpret it as a crossover from quantum to classical behavior.

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I. INTRODUCTION

The spin 1/2 XXZ spin chain

$$H = \frac{1}{2}\Sigma_{j=0}^{N-1}(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\sigma_j^z\sigma_{j+1}^z) \tag{1.1}$$

was first exactly studied by Bethe[1] in 1931 for $\Delta = \pm 1$, extensively investigated for $\Delta = 0$ in 1960 by Lieb, Schultz and Mattis[2] and studied for general values of Δ in 1966 by Yang and Yang[3]-[5]. Since these initial studies the thermodynamics have been extensively investigated[6] and by now are fairly well understood. The spin-spin correlations, however, are much more difficult to study and even the simplest of the equal time correlations

$$S^z(n;T,\Delta) = \mathrm{Tr}\sigma_0^z\sigma_n^z e^{-H/kT}/\mathrm{Tr}e^{-H/kT} \tag{1.2}$$

is only partially understood after decades of research[2,7]-[29]. In this note we extend these investigations of $S^z(n;T,\Delta)$ for $T > 0$ by means of an exact computer diagonalization of chains of $N = 16$ and 18 spins for $-1 \leq \Delta \leq 0$. Our results are presented below in tables 1-7 and Figs. 1 and 2. In the remainder of this note we discuss the significance and the interpretation of these results.

II. RESULTS AND DISCUSSION

The correlation $S^z(n;T,0)$ for the case $\Delta = 0$ was exactly computed long ago[2] to be

$$S^z(n;T,0) = \begin{cases} -[\frac{1}{\pi}\int_0^\pi d\phi \sin(n\phi)\tanh(\frac{1}{kT}\sin\phi)]^2 & \text{if } n \text{ is odd} \\ \delta_{n,0} & \text{if } n \text{ is even.} \end{cases} \tag{2.1}$$

This correlation is manifestly never positive for $n \neq 0$. When $T = 0$ it simplifies to

$$S^z(n;0,0) = \begin{cases} -4\pi^{-2}n^{-2} & \text{if } n \text{ is odd} \\ \delta_{n,0} & \text{if } n \text{ is even.} \end{cases} \tag{2.2}$$

In the scaling limit where

$$T \to 0, \quad n \to \infty, \quad \text{with } \; Tn = r \; \text{ fixed} \tag{2.3}$$

we have[8]

$$\lim T^{-2} S^z(n;T,0) = \begin{cases} -\sinh^{-2}(\pi r/2) & \text{if } n \text{ is odd} \\ 0 & \text{if } n \text{ is even.} \end{cases} \tag{2.4}$$

In the general case $\Delta \neq 0$ the nearest neighbor correlation at $T = 0$ $S^z(1;0,\Delta)$ is obtained from the derivative of the ground state energy[4] with respect to Δ. This correlation is negative for $-1 < \Delta$ and is plotted in Fig. 3 of ref[9]. For large n the behavior of $S^z(n;0,\Delta)$ at $T = 0$ has been extensively investigated and for $|\Delta| < 1$ we have[10,11] for $n \to \infty$

$$S^z(n,;0,\Delta) \sim -\frac{1}{\pi^2 \theta n^2} + (-1)^n \frac{C(\Delta)}{n^{\frac{1}{\theta}}} \tag{2.5}$$

where from ref.[9]

$$\theta = \frac{1}{2} + \frac{1}{\pi} \arcsin \Delta. \tag{2.6}$$

We note that $0 \leq \theta \leq 1$ and vanishes at the ferromagnetic point $\Delta = -1$. At $\Delta = 0$ we have $\theta = 1/2,\ C(0) = 2\pi^{-2}$ and (2.5) reduces to the exact result (2.4). For other values of Δ only the limiting value as $\Delta \to 1$ is known[28].

When $T > 0$ the correlations decay exponentially for large n instead of the algebraic decay (2.5) of $T = 0$. For $0 < \Delta < 1$ it is known[17,19] that for small fixed positive T the large n behavior of $S^z(n;T,\Delta)$ is

$$S^z(n;T,\Delta) \sim A_z(\Delta,T)(-1)^n e^{-nkT\pi(1-\theta)\theta^{-1}(1-\Delta^2)^{-1/2}}. \tag{2.7}$$

In order to smoothly connect to the $T = 0$ result (2.5) we need $A_z(\Delta,T) = A(\Delta)T^{1/\theta}$ but this has not yet been demonstrated. We note that for positive values of Δ the exact nearest neighbor correlation at $T = 0$ is negative and the leading term in the asymptotic behaviors (2.5) and (2.7) oscillates as $(-1)^n$. Both of these facts are consistent with antiferromagnetism.

For negative values of Δ, however, the situation is somewhat different. The nearest neighbor correlation at $T = 0$ is negative and, indeed, since $\theta < 1/2$, we see from (2.5) that the asymptotic values of $S^z(n;0,\Delta)$ are also negative and there are no oscillations. This behavior cannot be called antiferromagnetic because there are no oscillations but neither can it be called ferromagnetic because the correlations are negative instead of positive.

In order to further investigate the regime $-1 < \Delta < 0$ we have computed the correlation function $S^z(n; T, \Delta)$ by means of exact diagonalization for systems of $N = 16$ and $N = 18$ spins. Our results for $N = 18$ with $\Delta = -.1, -.3, -.9$ and -1.0 are given in tables 1-4 where we give $S^z(n; T, \Delta)$ for $1 \leq n \leq 8$ and $\frac{1}{2}S^z(n; T, \Delta)$ for $n = 9$. The factor of 1/2 for $n = 9$ is used because for $n = N/2$ there are two paths of equal length joining 0 and n in the finite system whereas for the same n in the infinite size system there will be only one path of finite length. To estimate the precision with which the $N = 18$ system gives the $N = \infty$ correlations we give in table 5 the correlation for $N = 16$ and $\Delta = -0.9$. We see here that for $T \geq .5$ the $N = 18$ correlations are virtually identical with the $N = 16$ correlations. Even for $T = .1$ and $T = .2$ the $N = 18$ data should be qualitatively close to the $N = \infty$ values.

The tables 1-5 reveal for $-1 \leq \Delta \leq 0$ the striking property that $S^z(n; T, \Delta)$, which is always negative at $T = 0$, becomes positive for fixed n at sufficiently large T. We study this further in table 6 where we list the values $T_0(n; \Delta)$ where $S^z(n; T_0(n; \Delta), \Delta) = 0$. This table indicates that

$$\lim_{n\to\infty} T_0(n; \Delta) > 0. \tag{2.8}$$

We denote this limiting temperature by $T_0(\Delta)$ and note that this implies that in the expansion of $S^z(n; T, \Delta)$ obtained from the quantum transfer matrix formalism[17]

$$S^z(n; T, \Delta) = \sum_{j=1} C_j(T; \Delta) e^{-n\gamma_j(T)} \quad \text{with } \gamma_j < \gamma_{j+1} \tag{2.9}$$

we have $C_1(T_0(\Delta); \Delta) = 0$. If, for large n, we retain only the first two terms in the expansion, ignore the T dependence of $\gamma_j(T)$ and $C_2(T; \Delta)$ and write $C_1(T; \Delta) = (T - T_0(\Delta))C_1(\Delta)$ we see that the large n behavior of $T_0(n; \Delta)$ may be estimated as

$$T_0(n, \Delta) = T_0(\Delta) + Ae^{-n\gamma}. \tag{2.10}$$

where $\gamma = \gamma_2 - \gamma_1$ and $A = -C_2/C_1$. In Fig. 1 plot the data of table 6 versus a least squares fit using (2.10) and find that the fit is exceedingly good even for small n. The values of the

fitting parameters are given in table 7 for $-.9 \leq \Delta \leq -.1$ and $T_0(\Delta)$ is plotted in Fig. 2. The existence of this $T_0(\Delta) > 0$ for $-1 < \Delta < 0$ is quite different from the case $0 < \Delta < 1$ where for all temperatures the sign of $S^z(n; T, \Delta)$ is $(-1)^n$.

To interpret the property of changing sign we note that, when the Hamiltonian (1.1) is written in terms of the basis where σ_j^z is diagonal ($\sigma_j^z = \pm 1$), the term $\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y$ is a kinetic energy term which translates a down spin one step whereas the term $\sigma_j^z \sigma_{j+1}^z$ is a potential energy term which is diagonal in the basis of eigenstates of σ_j^z. In classical statistical mechanics the static expectation values of position dependent operators are independent of the kinetic energy and depend only on the potential energy. If we further expect that at high temperatures the system should behave in a classical fashion we infer that at high temperatures for $\Delta < 0$ the correlation $S^z(n; T, \Delta)$ should be ferromagnetically aligned ie. $S^z(n; T, \Delta) > 0$. This is indeed what is seen in tables 1-5. However at low temperatures the quantum effects of the kinetic term cannot be ignored. When $\Delta = 0$ there is no potential energy so all the behavior in $S^z(n; T, 0)$ can only come from the kinetic terms and hence the behavior given by (2.1) in which $S^z(n; T, 0)$ is never positive for $n \neq 0$ must be purely quantum mechanical. Consequently it seems appropriate to refer to the change of sign of the correlation $S^z(n; T, \Delta)$ as a quantum to classical crossover.

The low temperature behavior of the correlation function is determined by conformal field theory. In particular we consider the scaling limit (2.3) and define the scaling function

$$f(r, \Delta) = \lim T^{-2} S^z(n; T, \Delta). \tag{2.11}$$

The prescription of conformal field theory is that this scaling function is obtained from the large n behavior of the $T = 0$ correlation given by the first term of (2.5) by the replacement [page 513 of ref.[19]]

$$n \rightarrow (\kappa T/2)^{-1} \sinh \kappa r/2 \tag{2.12}$$

where the decay constant κ can be obtained by use of the methods of ref.[17]. This replacement is obtained by combining the conformal field theory results on finite size corrections[30] with

the field theory relation of finite strip size to nonzero temperature[31]. This prescription clearly leads to a correlation which is always negative and does not show the sign changing phenomena seen in the tables 1-5. However, this result is only a limiting result as $T \rightarrow 0$. The results of this paper indicate that there is further physics in the high temperature behavior of the XXZ chain where $T > T_0(\Delta)$ which is not contained in this conformal field theory result.

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TABLES

T	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$	$n=9$
0.1	−3.81e-01	−1.87e-02	−3.74e-02	−4.51e-03	−1.19e-02	−2.01e-03	−5.81e-03	−1.28e-03	−2.21e-03
0.2	−3.69e-01	−1.75e-02	−2.82e-02	−3.13e-03	−5.72e-03	−8.43e-04	−1.47e-03	−2.99e-04	−3.51e-04
0.5	−2.78e-01	−1.10e-02	−5.88e-03	−4.65e-04	−2.27e-04	−2.24e-05	−9.31e-06	−1.11e-06	−3.86e-07
1.0	−1.29e-01	−3.25e-03	−3.25e-04	−1.28e-05	−1.18e-06	−5.28e-08	−4.43e-09	−2.15e-10	−1.67e-11
2.0	−3.25e-02	−3.49e-04	−3.92e-06	−9.71e-09	3.34e-10	1.01e-11	<1.0e-12	<1.0e-12	<1.0e-12
3.0	−1.02e-02	−2.76e-05	4.84e-07	9.49e-09	8.85e-11	<1.0e-12	<1.0e-12	<1.0e-12	<1.0e-12
4.0	−2.91e-03	2.53e-05	4.85e-07	4.45e-09	3.05e-11	<1.0e-12	<1.0e-12	<1.0e-12	<1.0e-12
5.0	6.54e-05	3.26e-05	3.44e-07	2.44e-09	1.54e-11	<1.0e-12	<1.0e-12	<1.0e-12	<1.0e-12
10.0	2.50e-03	1.66e-05	7.47e-08	3.09e-10	1.28e-12	<1.0e-12	<1.0e-12	<1.0e-12	<1.0e-12
20.0	1.87e-03	5.20e-06	1.21e-08	2.77e-11	<1.0e-12	<1.0e-12	<1.0e-12	<1.0e-12	<1.0e-12

TABLE I. The correlation $(1-\frac{1}{2}\delta_{n,N/2})S^z(n;T,\Delta)$ for $\Delta=-.1$ for the XXZ spin chain with $N=18$ sites.

T	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$	$n=9$
0.1	−3.35e-01	−5.19e-02	−3.23e-02	−1.08e-02	−9.19e-03	−4.14e-03	−3.93e-03	−2.32e-03	−1.39e-03
0.2	−3.17e-01	−4.71e-02	−2.25e-02	−6.41e-03	−3.64e-03	−1.28e-03	−7.22e-04	−3.19e-04	−1.38e-04
0.5	−1.97e-01	−2.13e-02	−3.09e-03	−3.32e-04	−3.77e-05	−2.78e-06	−1.70e-07	1.06e-08	3.20e-09
1.0	−5.27e-02	−8.92e-04	2.04e-04	3.00e-05	2.38e-06	1.33e-07	6.04e-09	3.33e-10	2.95e-11
2.0	1.40e-02	2.18e-03	1.49e-04	7.98e-06	4.09e-07	2.16e-08	1.16e-09	6.30e-11	3.37e-12
3.0	2.20e-02	1.47e-03	6.52e-05	2.60e-06	1.04e-07	4.19e-09	1.70e-10	6.87e-12	<1.0e-12
4.0	2.16e-02	9.76e-04	3.29e-05	1.05e-06	3.34e-08	1.07e-09	3.45e-11	1.11e-12	<1.0e-12
5.0	1.98e-02	6.82e-04	1.87e-05	4.92e-07	1.30e-08	3.47e-10	9.22e-12	<1.0e-12	<1.0e-12
10.0	1.25e-02	1.99e-04	2.83e-06	4.00e-08	5.65e-10	8.00e-12	<1.0e-12	<1.0e-12	<1.0e-12
20.0	6.87e-03	5.30e-05	3.87e-07	2.82e-09	2.06e-11	<1.0e-12	<1.0e-12	<1.0e-12	<1.0e-12

TABLE II. The correlation $(1-\frac{1}{2}\delta_{n,N/2})S^z(n;T,\Delta)$ for $\Delta=-.3$ for the XXZ spin chain with $N=18$ sites.

T	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$	$n=9$
0.1	−5.46e-02	−2.14e-02	−3.41e-03	5.10e-03	8.06e-03	8.19e-03	7.27e-03	6.35e-03	2.99e-03
0.2	8.19e-02	8.50e-02	7.12e-02	5.22e-02	3.51e-02	2.26e-02	1.47e-02	1.05e-02	4.61e-03
0.5	2.02e-01	1.36e-01	7.38e-02	3.62e-02	1.72e-02	8.18e-03	4.03e-03	2.23e-03	8.66e-04
1.0	2.05e-01	8.74e-02	3.03e-02	9.96e-03	3.26e-03	1.07e-03	3.56e-04	1.28e-04	3.81e-05
2.0	1.55e-01	3.57e-02	7.11e-03	1.39e-03	2.72e-04	5.33e-05	1.05e-05	2.13e-06	4.01e-07
3.0	1.19e-01	1.83e-02	2.55e-03	3.51e-04	4.83e-05	6.66e-06	9.19e-07	1.29e-07	1.75e-08
4.0	9.51e-02	1.10e-02	1.17e-03	1.24e-04	1.31e-05	1.39e-06	1.48e-07	1.58e-08	1.66e-09
5.0	7.90e-02	7.29e-03	6.28e-04	5.40e-05	4.64e-06	3.99e-07	3.43e-08	2.97e-09	2.53e-10
10.0	4.23e-02	1.94e-03	8.53e-05	3.76e-06	1.66e-07	7.30e-09	3.22e-10	1.42e-11	<1.0e-12
20.0	2.19e-02	4.96e-04	1.11e-05	2.46e-07	5.48e-09	1.22e-10	2.72e-12	<1.0e-12	<1.0e-12

TABLE III. The correlation $(1-\frac{1}{2}\delta_{n,N/2})S^z(n;T,\Delta)$ for $\Delta=-.9$ for the XXZ spin chain with $N=18$ sites.

T	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$	$n=9$
0.1	3.30e-01	3.19e-01	3.02e-01	2.83e-01	2.64e-01	2.47e-01	2.33e-01	2.25e-01	1.11e-01
0.2	3.21e-01	2.87e-01	2.41e-01	1.95e-01	1.55e-01	1.25e-01	1.05e-01	9.28e-02	4.45e-02
0.5	2.95e-01	2.04e-01	1.21e-01	6.74e-02	3.70e-02	2.06e-02	1.19e-02	7.78e-03	3.28e-03
1.0	2.50e-01	1.14e-01	4.41e-02	1.63e-02	6.04e-03	2.24e-03	8.46e-04	3.50e-04	1.14e-04
2.0	1.79e-01	4.50e-02	9.99e-03	2.19e-03	4.79e-04	1.05e-04	2.31e-05	5.30e-06	1.11e-06
3.0	1.35e-01	2.29e-02	3.55e-03	5.46e-04	8.40e-05	1.29e-05	1.99e-06	3.14e-07	4.72e-08
4.0	1.07e-01	1.37e-02	1.62e-03	1.92e-04	2.27e-05	2.68e-06	3.17e-07	3.80e-08	4.43e-09
5.0	8.88e-02	9.06e-03	8.70e-04	8.33e-05	7.99e-06	7.65e-07	7.33e-08	7.09e-09	6.73e-10
10.0	4.73e-02	2.40e-03	1.18e-04	5.77e-06	2.83e-07	1.39e-08	6.81e-10	3.35e-11	1.64e-12
20.0	2.44e-02	6.13e-04	1.52e-05	3.77e-07	9.33e-09	2.31e-10	5.73e-12	<1.0e-12	<1.0e-12

TABLE IV. The correlation $(1-\frac{1}{2}\delta_{n,N/2})S^z(n;T,\Delta)$ for $\Delta=-1.0$ for the XXZ spin chain with $N=18$ sites.

T	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$
0.1	−5.62e-02	−2.25e-02	−4.06e-03	4.90e-03	8.37e-03	9.12e-03	8.91e-03	4.37e-03
0.2	7.92e-02	8.32e-02	7.02e-02	5.20e-02	3.56e-02	2.40e-02	1.74e-02	7.65e-03
0.5	2.02e-01	1.36e-01	7.38e-02	3.63e-02	1.73e-02	8.49e-03	4.70e-03	1.82e-03
1.0	2.05e-01	8.74e-02	3.03e-02	9.96e-03	3.26e-03	1.08e-03	3.90e-04	1.16e-04
2.0	1.55e-01	3.57e-02	7.11e-03	1.39e-03	2.72e-04	5.34e-05	1.08e-05	2.05e-06
3.0	1.19e-01	1.83e-02	2.55e-03	3.51e-04	4.83e-05	6.66e-06	9.36e-07	1.27e-07
4.0	9.51e-02	1.10e-02	1.17e-03	1.24e-04	1.31e-05	1.39e-06	1.49e-07	1.56e-08
5.0	7.90e-02	7.29e-03	6.28e-04	5.40e-05	4.64e-06	3.99e-07	3.45e-08	2.95e-09
10.0	4.23e-02	1.94e-03	8.53e-05	3.76e-06	1.66e-07	7.30e-09	3.23e-10	1.42e-11
20.0	2.19e-02	4.96e-04	1.11e-05	2.46e-07	5.48e-09	1.22e-10	2.72e-12	<1.0e-12

TABLE V. The correlation $(1-\frac{1}{2}\delta_{n,N/2})S^z(n;T,\Delta)$ for $\Delta=-.9$ for the XXZ spin chain with $N=16$ sites.

Δ	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$	$n=9$
−0.1	4.966	3.323	2.561	2.073	1.870	1.706	1.669	1.592	
−0.2	2.432	1.643	1.275	1.037	0.923	0.840	0.811	0.774	0.767
−0.3	1.561	1.071	0.839	0.687	0.602	0.545	0.517	0.493	0.483
−0.4	1.103	0.771	0.612	0.505	0.437	0.392	0.365	0.346	0.335
−0.5	0.807	0.578	0.464	0.388	0.334	0.297	0.272	0.253	0.243
−0.6	0.589	0.434	0.355	0.300	0.259	0.229	0.206	0.189	0.180
−0.7	0.413	0.318	0.264	0.227	0.198	0.175	0.156	0.140	0.132
−0.8	0.265	0.215	0.184	0.161	0.142	0.126	0.112	0.099	0.094
−0.9	0.137	0.118	0.104	0.092	0.082	0.073	0.065	0.059	0.057

TABLE VI. The values of $T_0(n;\Delta)$ at which the correlation function $S^z(n;T_0(n;\Delta),\Delta)$ vanishes for $N=18$

Δ	T_0	γ	A
-0.1	1.550	0.585	5.734
-0.2	0.745	0.547	2.690
-0.3	0.462	0.491	1.630
-0.4	0.312	0.433	1.093
-0.5	0.216	0.374	0.764
-0.6	0.148	0.317	0.539
-0.7	0.095	0.259	0.372
-0.8	0.054	0.205	0.241
-0.9	0.031	0.180	0.125

TABLE VII. The fitting parameters T_0, γ and A of (2.10) for $\Delta = -.1, \cdots, -.9$

Figure Captions

Figure 1. A plot of the exact zeroes $T_0(n; \Delta)$ of the $N = 18$ system compared with the fitting form (2.9). The values $\Delta = -.1, \cdots, -.9$ are given with $\Delta = -.1$ being the highest.

Figure 2. The temperature $T_0(\Delta)$ plotted as a function of Δ.

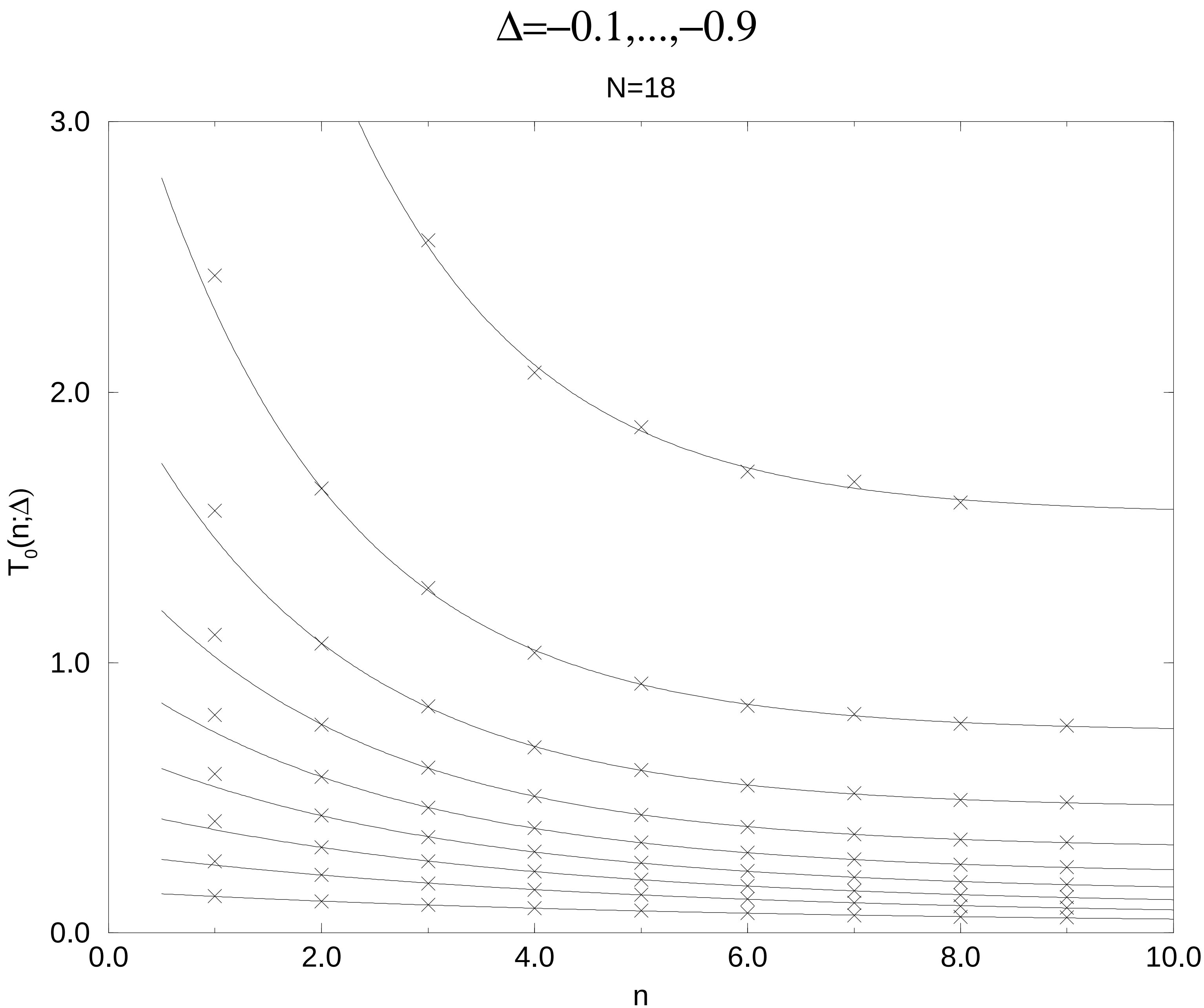

Fig. 1

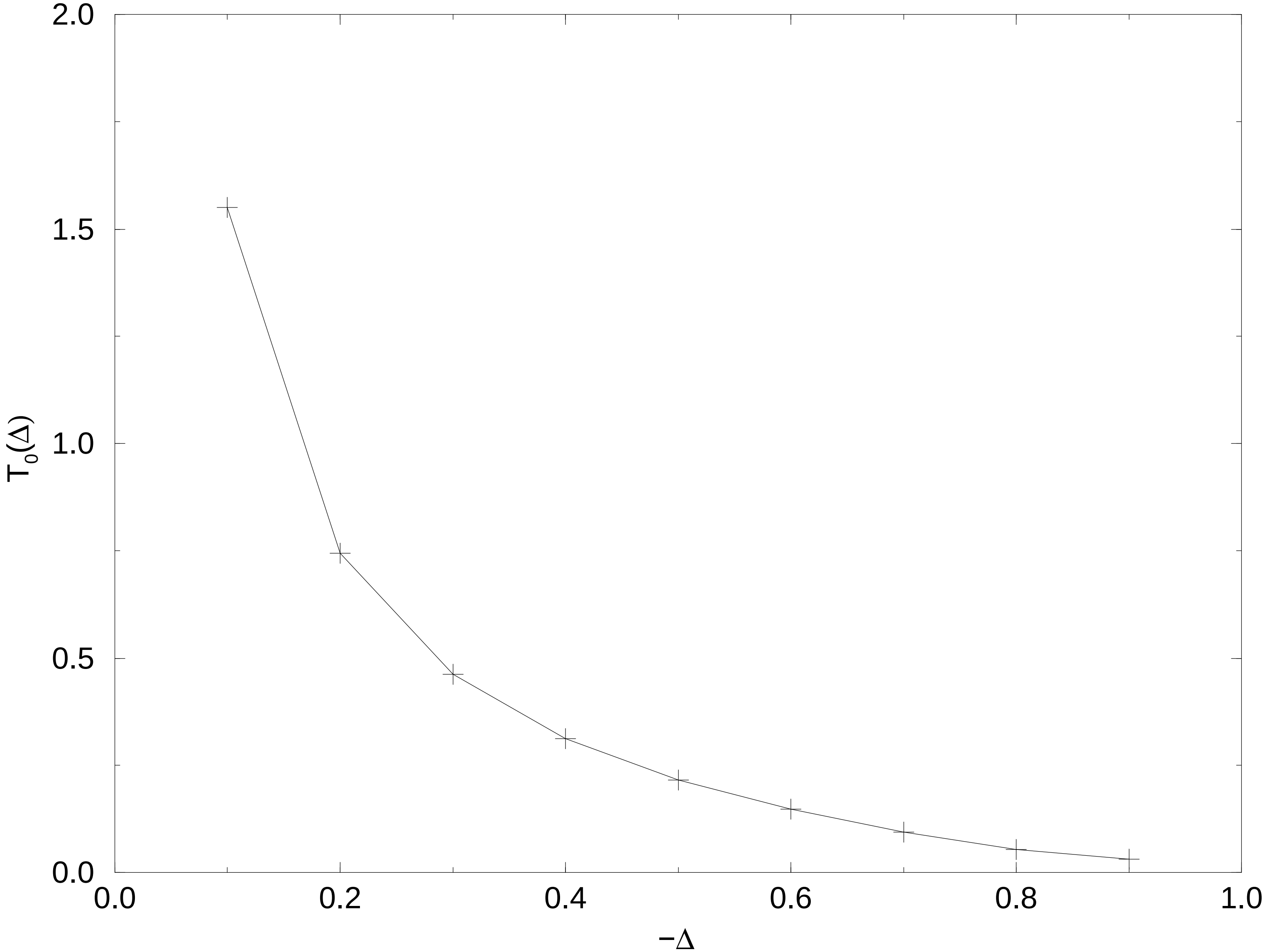

Fig. 2

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